Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

Project ID: ACS015

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June 20th, 2018

DOE Management Team
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Project Overview

Budget

- FY17: $300k
- FY18: $300k

(~ 0.5 FTE + materials)

Barriers

ACEC Roadmap, Topic Area 1

- Thermal management (efficient low-cost waste-heat recovery…)
- Increase EGR dilution tolerance
- Reduce content, cost, and complexity of engines while increasing efficiency

Timeline

- Part of ORNL's FY17-FY19 lab call
- New lab call beginning FY19, proposing continuing work
- Builds on prior Stretch Efficiency research program at ORNL
- Focus on thermochemical recuperation in 2011

Collaborators

- Ford – Providing technical input
- Caterpillar – Providing technical input
- FCA – Providing technical input
- AEC working group led by SNL
  - Industry feedback
- Aramco Services – Technical collaboration
- ANSYS (formerly Reaction design) – CFD model development
- Umicore – Catalyst coatings

Universities

- University of Michigan - Galen Fisher
- University of Michigan – Yan Chang

National Labs

- SNL - Isaac Ekoto

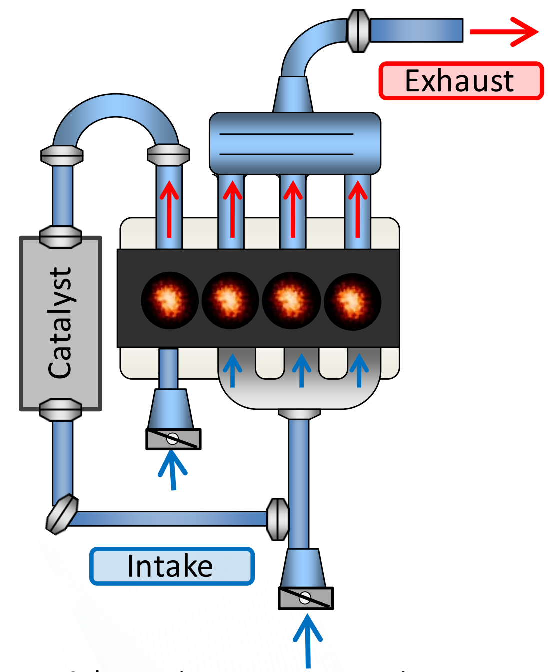
Relevance: Decreased Petroleum Consumption through Higher Engine Efficiency

Overall Project Goal

- Increase IC engine efficiency with an approach centered on thermodynamic of engine processes and minimizing losses

ACEC Roadmap, Area 1, Research Priorities Addressed

- Thermal management (efficient low-cost waste-heat recovery)
  - This project is investigating the feasibility of waste-heat recovery through thermochemical recuperation (TCR)
- Increase EGR dilution tolerance
  - EGR-loop catalytic reforming produces a H_2 and CO mixture capable of extending EGR dilution tolerance
  - EGR dilution tolerance approaching 50% demonstrated in 2017 AMR
- Reduce content, cost, and complexity of engines while increasing efficiency
  - Relative to lean-burn options for high efficiency, the stoichiometric approach here simplifies emissions control cost and complexity



Note: Schematic represents engine flow paths and is not intended to represent instrumentation or controls

This Project has Two Tracked Milestones for FY18

Second Quarter, FY2018

Perform a coarse engine map of engine operation (efficiency and emissions) with the catalytic reforming strategy from near-idle to boosted engine operating conditions.

Status: Milestone not completed on time. Delayed to Q4.

Fourth Quarter, FY2018

Complete an assessment of the Rh catalyst sulfur deactivation and the ability to regenerate the catalyst at engine-relevant conditions.

Status: On-track.

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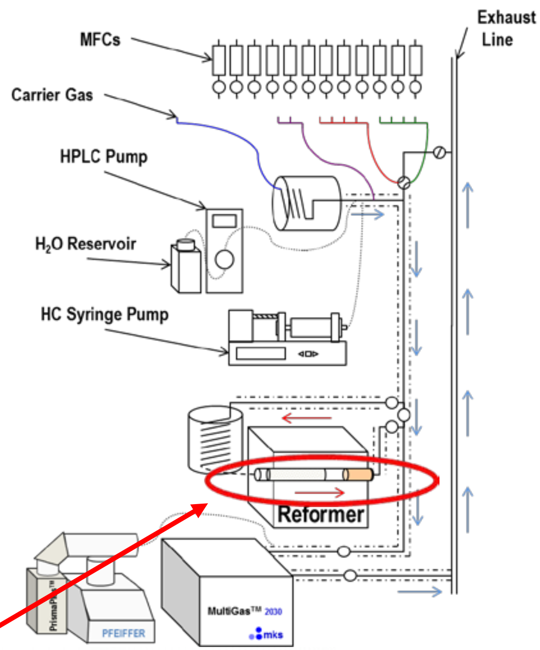
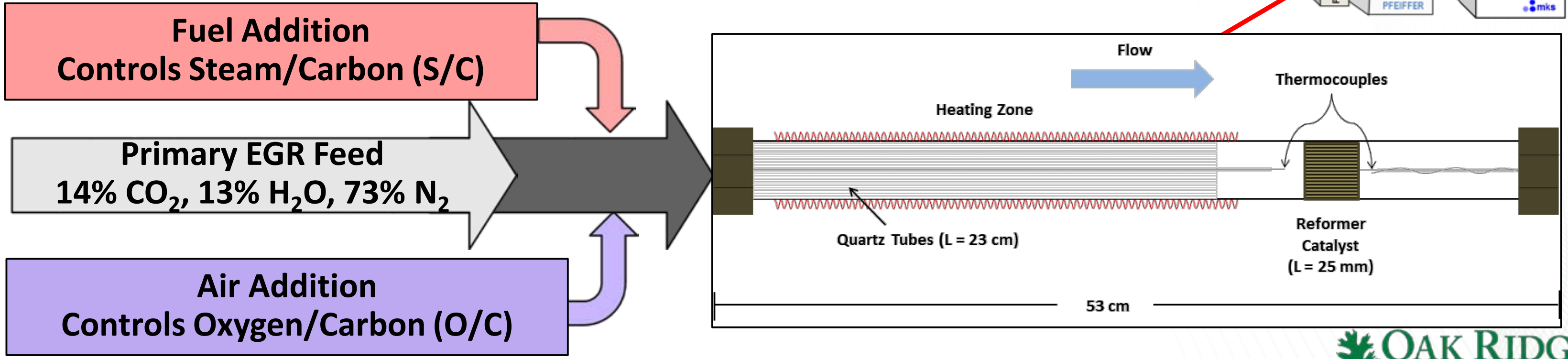
Synthetic Exhaust Flow Reactor Used to Guide Engine Investigations

- Steam and partial oxidation reforming investigated in an automated synthetic exhaust flow reactor for application in an EGR-loop reforming strategy on an SI engine
- Pre-commercial catalyst formulation from Umicore
  - 2 wt% Rh supported on Al_2O_3 and coated onto a zirconia-mullite substrate of 400 cells per square inch
- Identifies catalyst boundary conditions for efficient reforming, including thermochemical recuperation
  - Engine operated to mimic the catalyst boundary conditions
  - Excellent transferability has been demonstrated





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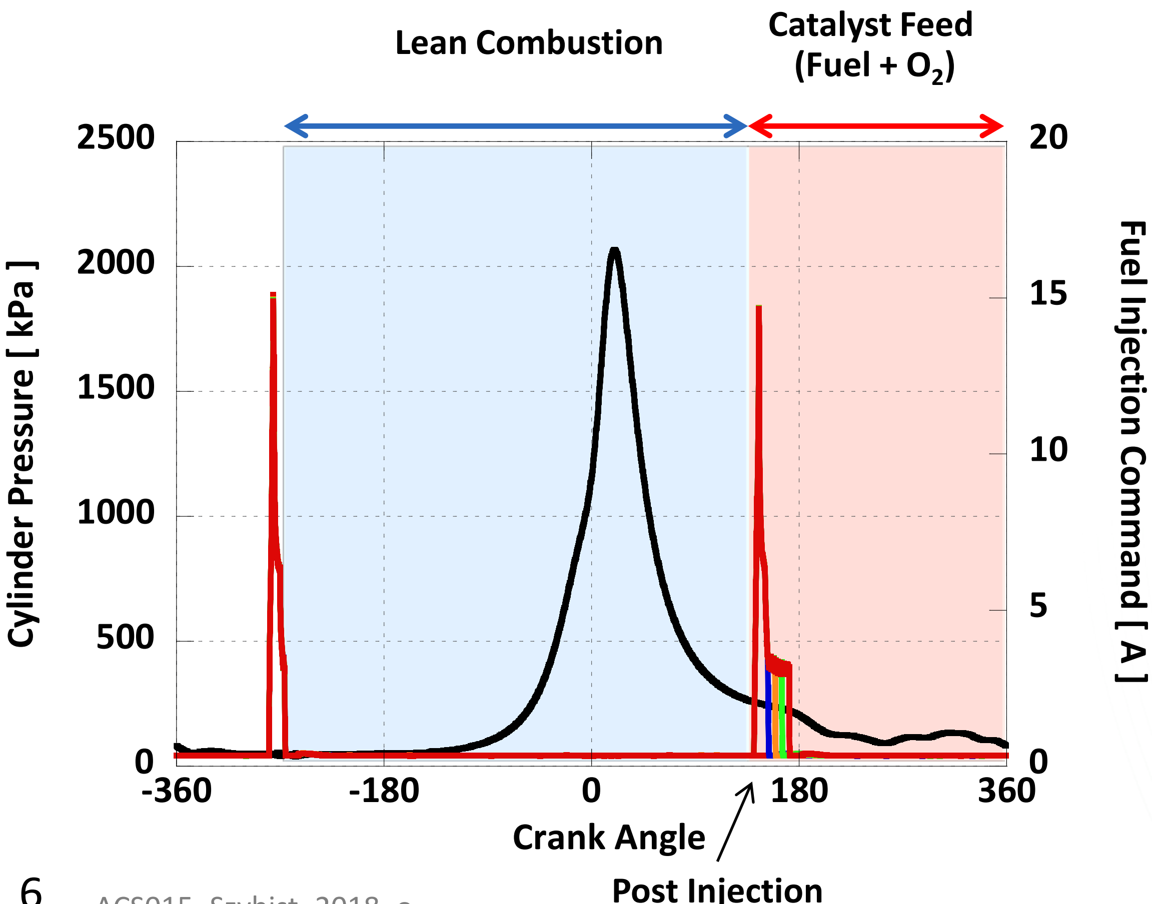
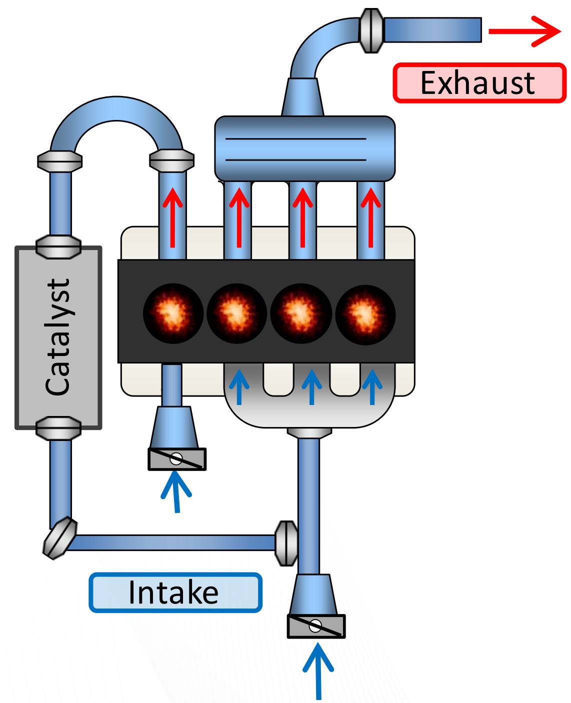
Implementation in an EGR Reforming Loop Requires Oxygen at the Reforming Catalyst

- Lean combustion by one cylinder to feed oxygen to reforming catalyst
  - Allows stoichiometric exhaust for 3-way exhaust TWC compatibility
  - Allows lean cylinder to be at a higher MAP, match load
- Fuel provided to catalyst through post injection event





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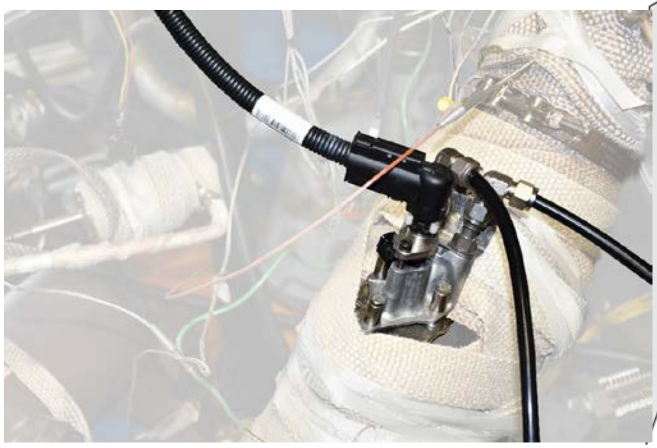
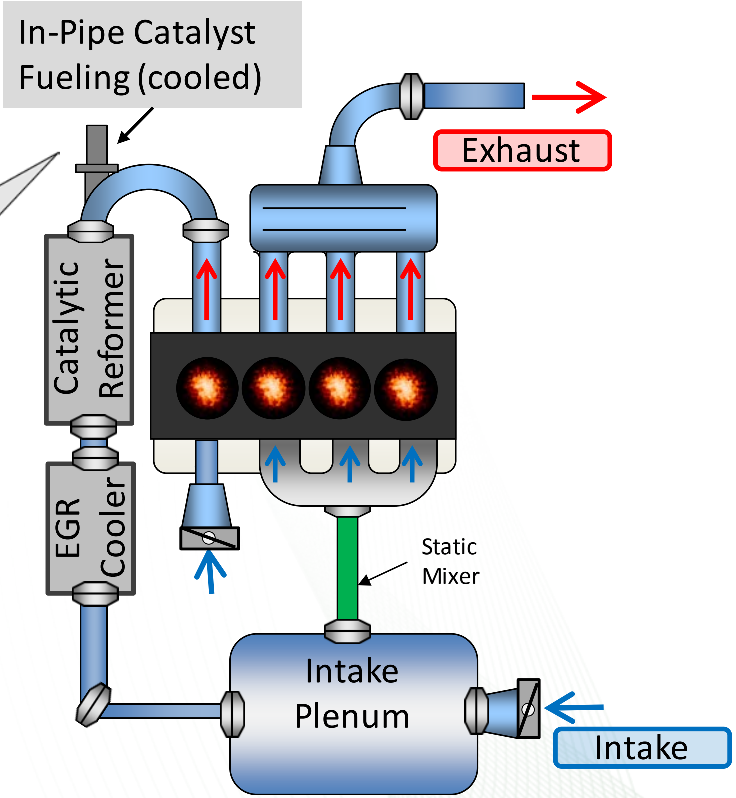
Implementation in an EGR Reforming Loop Requires Oxygen at the Reforming Catalyst

- Lean combustion by one cylinder to feed oxygen to reforming catalyst
  - Allows stoichiometric exhaust for 3-way exhaust TWC compatibility
  - Allows lean cylinder to be at a higher MAP, match load
- ~~Fuel provided to catalyst through post injection event~~
- In FY18, moved to in-pipe catalyst fueling using water-cooled PFI injector
  - Alleviates cylinder-to-cylinder load balancing
  - Alleviates oil dilution concerns





Three Studies Published in *Energy & Fuels* Detailing the Catalytic Reforming from Bench Flow Reactor to Full Engine System

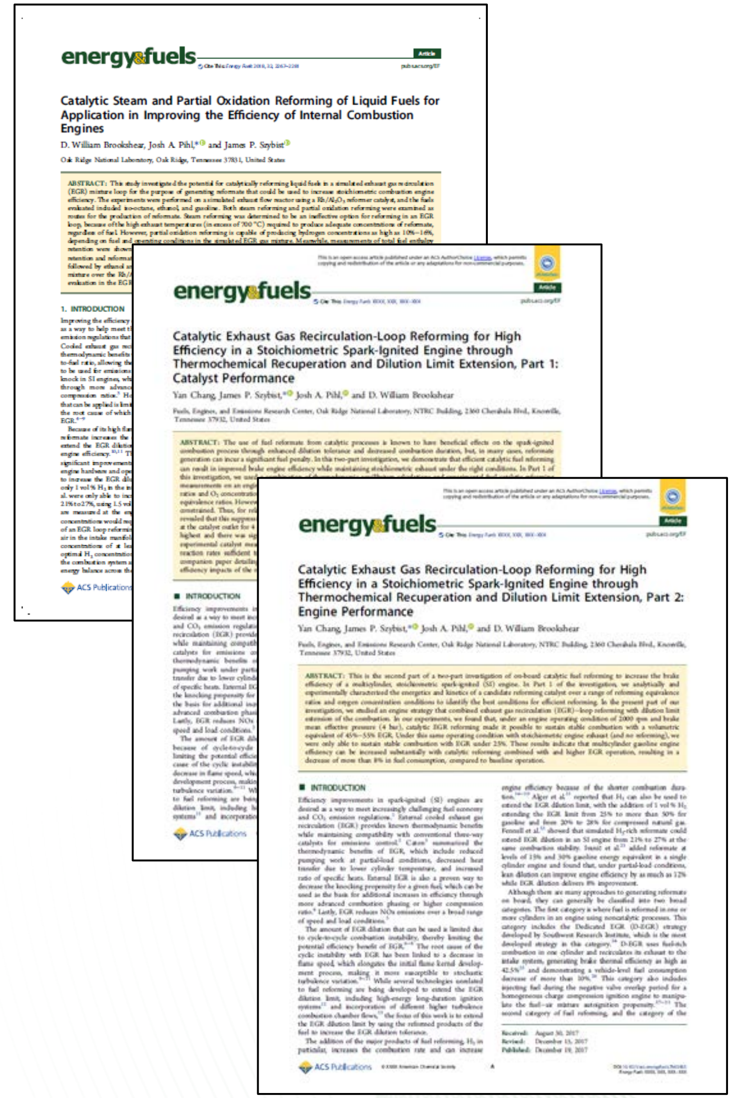
Accomplishments

- Results contained in these manuscripts presented at an early stage in 2017 DOE merit review
- Significant effort in analysis and reporting in the last year to publish manuscripts
- Combined, these tell a comprehensive story of developing efficient reforming conditions for engines

  Paper 1. Reforming using synthetic exhaust flow reactor.
  - Reforming performance and energy balances
  - Impact of different fuel compositions

  Paper 2. Catalyst performance on an engine with real exhaust
  - Reformate yield with real engine boundary conditions
  - Thermal conditions in catalyst and impact of water-gas shift reaction

  Paper 3. Full engine performance in multi-cylinder engine
  - Brake thermal efficiency gain
  - Impact of reformate on combustion processes
  - Comparison with conventional EGR



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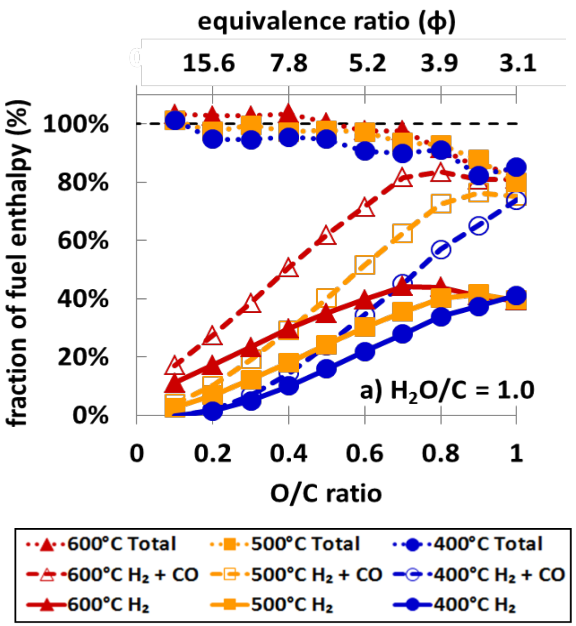
Efficient Reforming with Oxygen Present Requires Very Rich Conditions (Φ~7.0). Max H2 Production ≠ Max Efficiency.

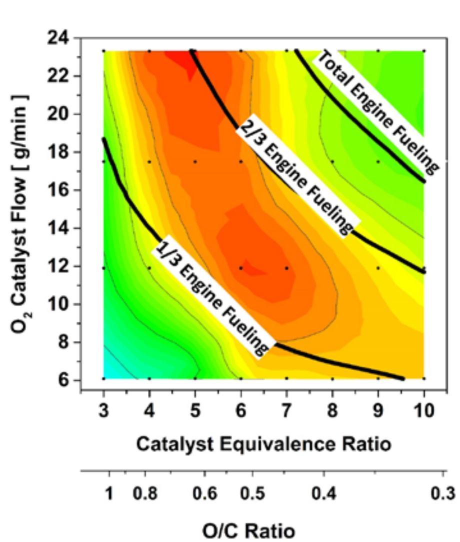
Accomplishments

Synthetic Exhaust Gas Flow Reactor Reforming Study



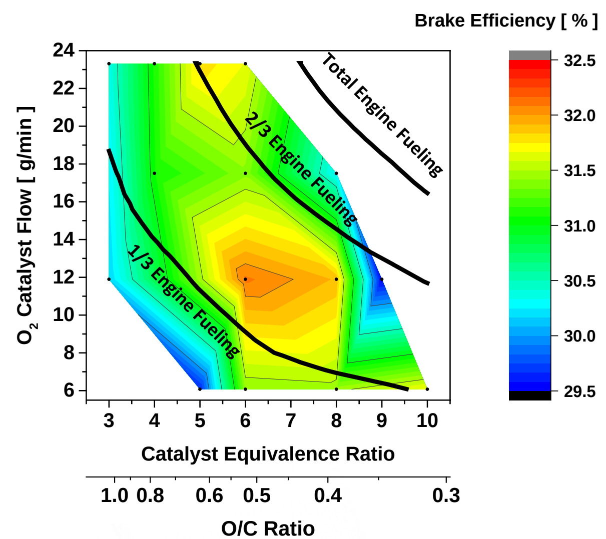
Efficient reforming and TCR requires Φ > 6. Energy balance dependent on inlet T.

Full-Sized Catalyst Performance Study On-Engine



Highest H_2 at Φ = 5-6, corresponded with significant water consumption (evidence of steam reforming reactions).

Multi-Cylinder Engine Performance Study with Reforming Strategy



Best brake efficiency occurred at minimum reforming oxygen concentration that produced high H_2 concentration.

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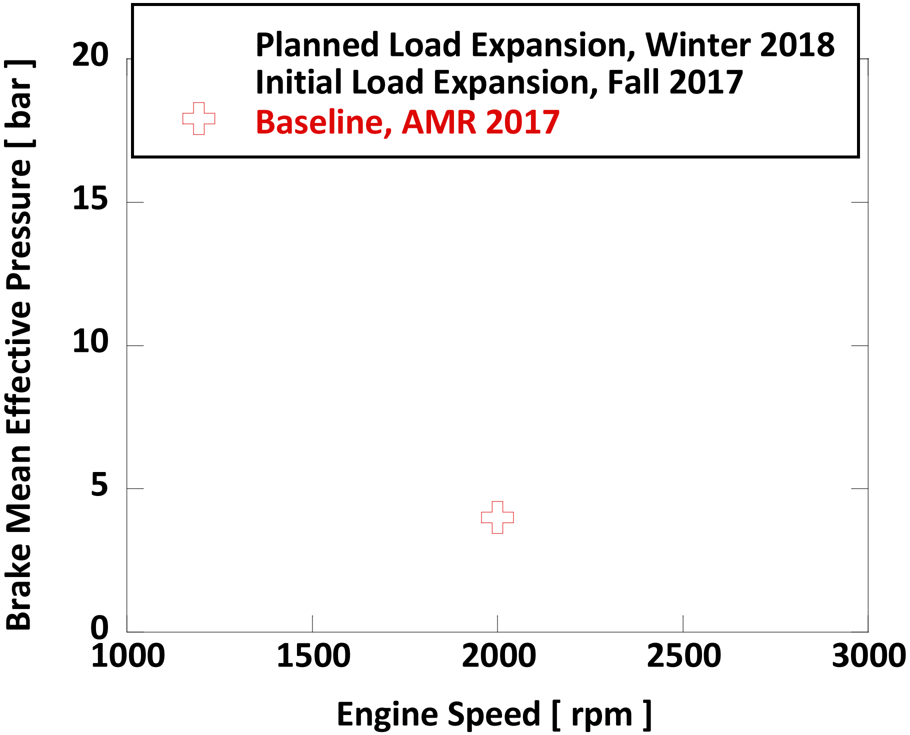
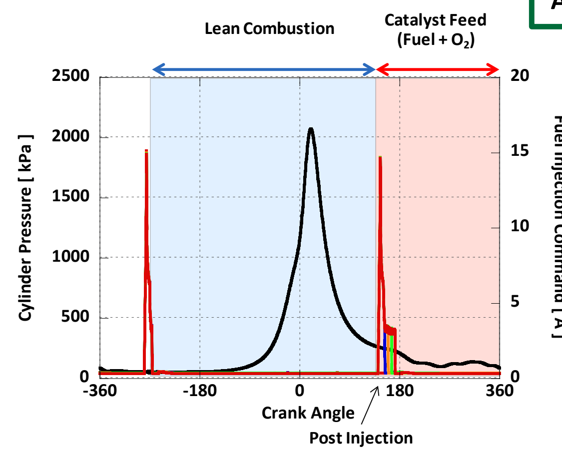
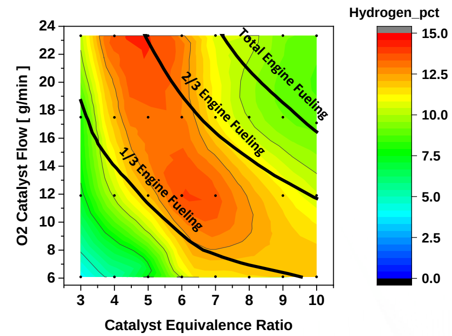
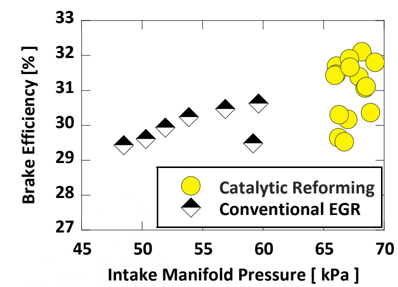
Significant Progress Made on Load Range Expansion, but Experimental Events Resulted in Equipment Failure. Goal Not Yet Met.









- Initial catalytic reforming engine investigation at 2000 rpm, 4 bar BMEP
  - Post-injection catalyst fueling strategy to efficient reforming boundary conditions
  - Hydrogen production of >15% catalyst-out, EGR tolerance >45%, fuel consumption decrease of 8%
  - Results presented at the 2017 AMR

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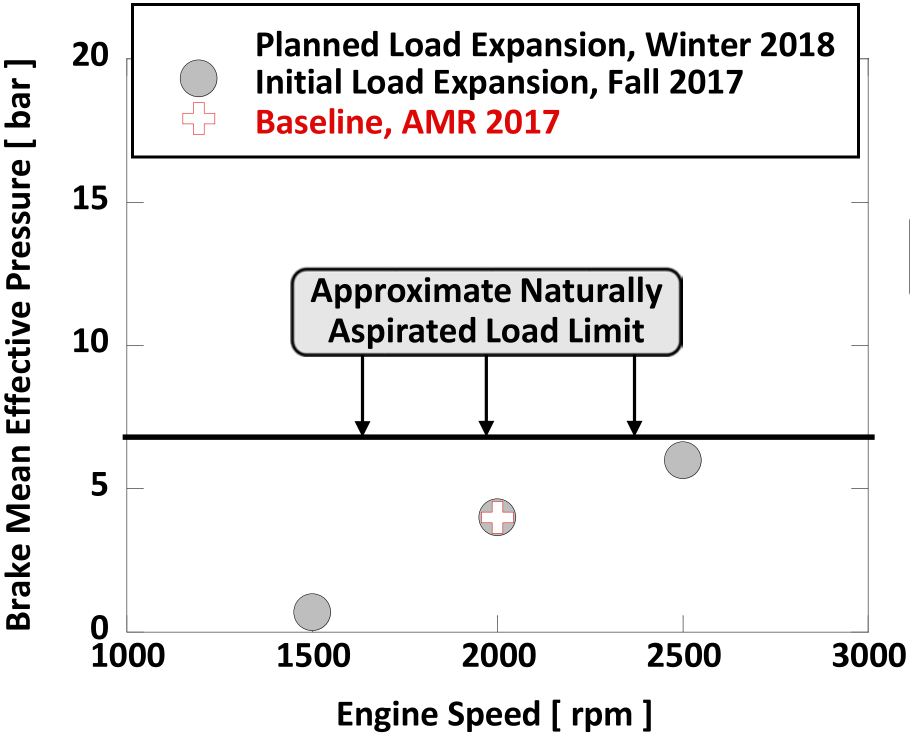
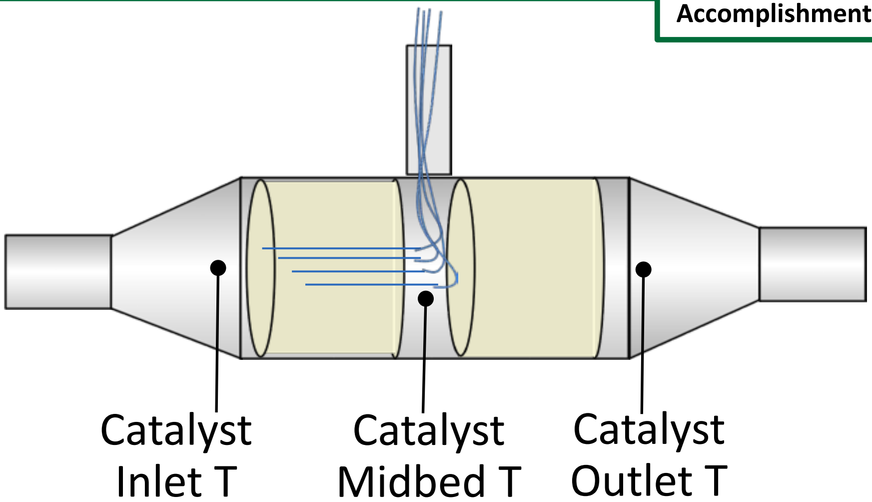
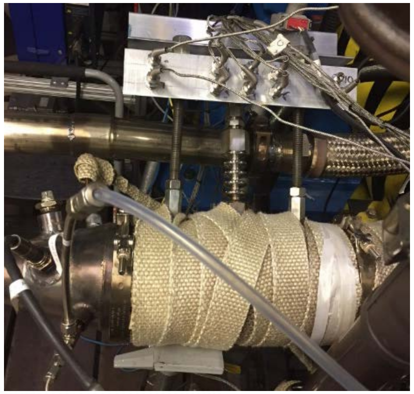


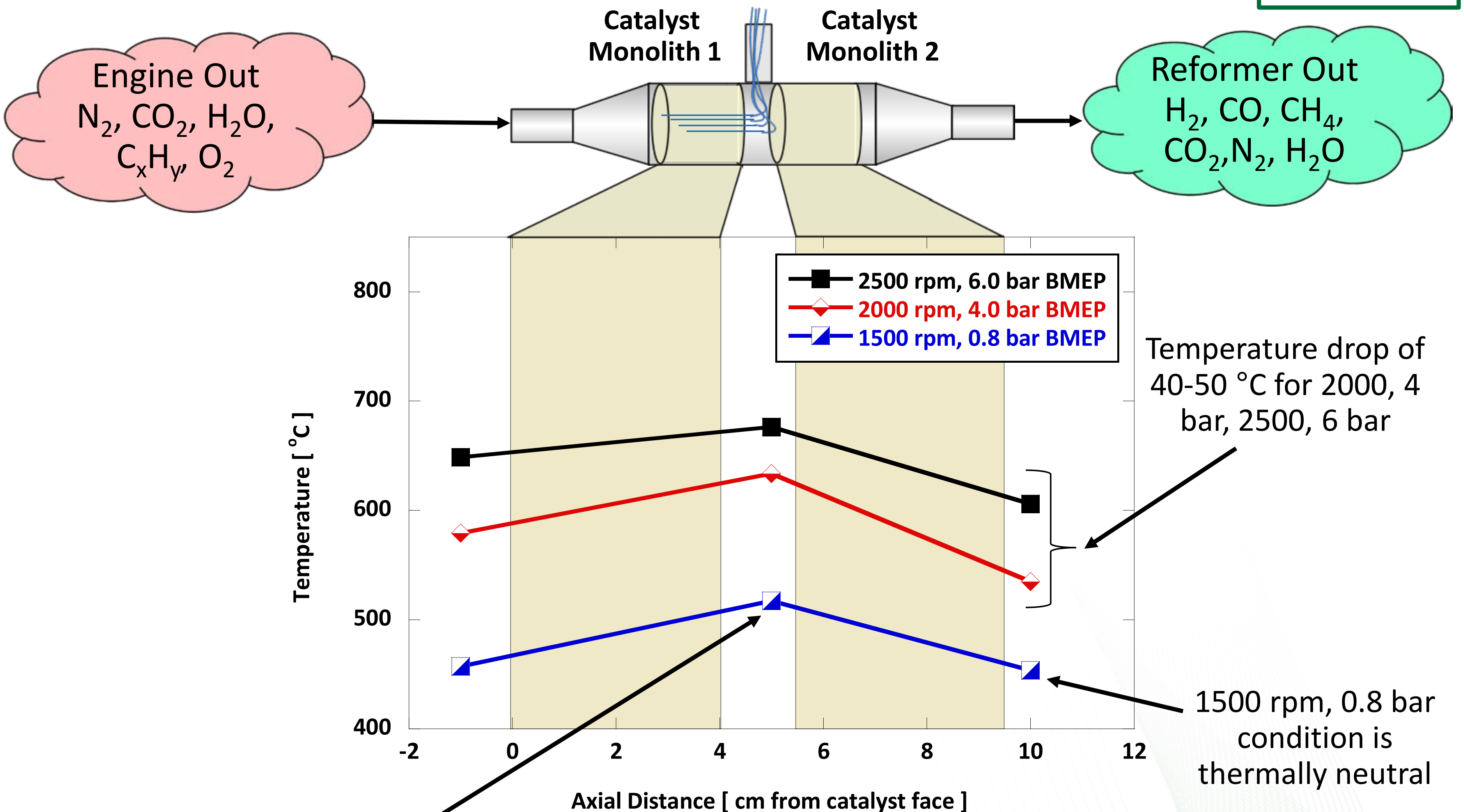




- Preliminary load range expansion accomplished Fall of 2017
  - Naturally aspirated load limit encountered at approximately 6 bar BMEP because of high dilution
  - Included nine thermocouples inside of catalyst to determine axial temperature profile
  - Unable to balance load between cylinders – particularly at the 1500 rpm, 0.7 bar BMEP point
- Hardware upgrades required for additional load range expansion

Axial Temperature Profiles for Preliminary Load Range Expansion Provide Confidence that Further Expansion is Possible

Accomplishments



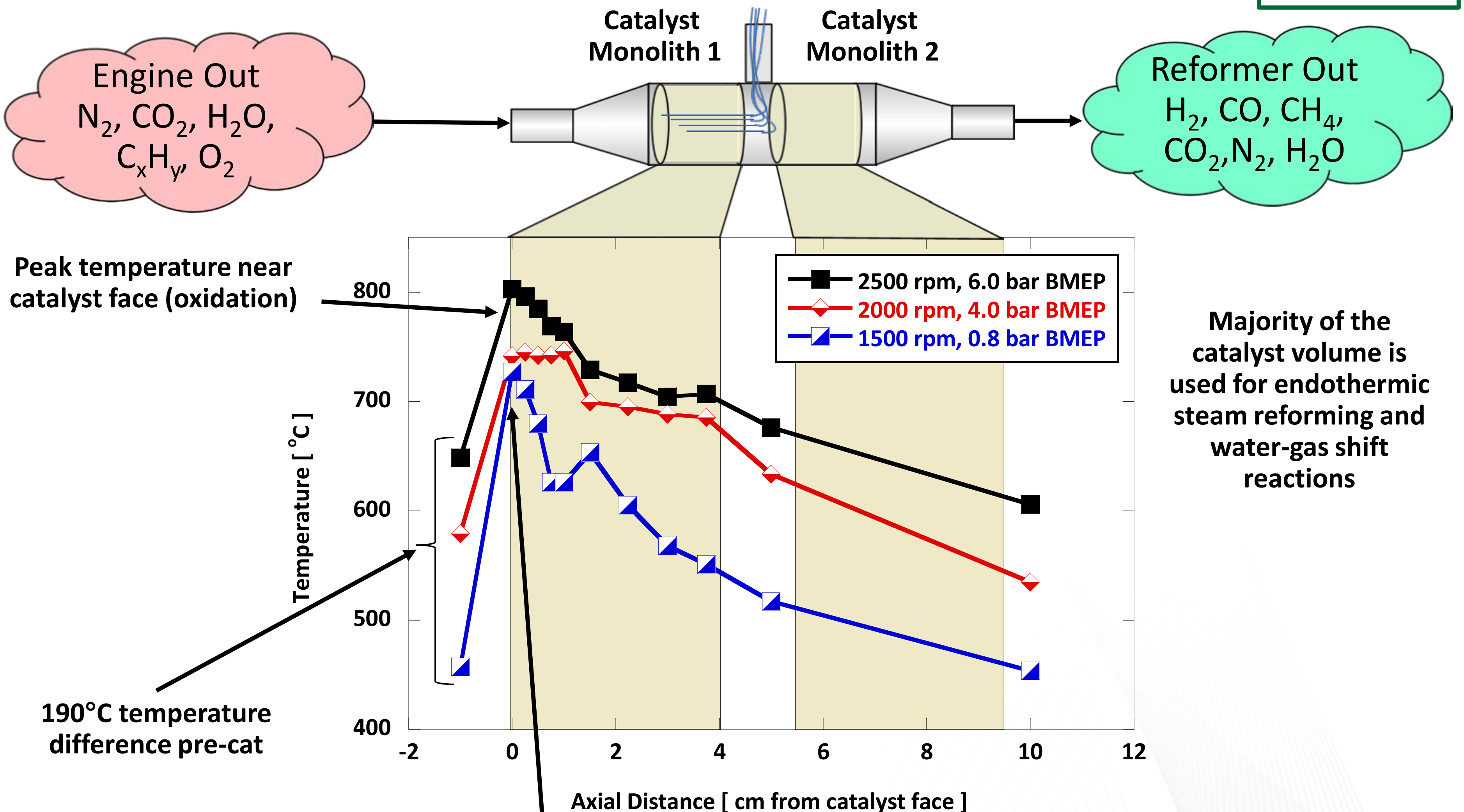
Temperature drop of 40-50 °C for 2000, 4 bar, 2500, 6 bar

1500 rpm, 0.8 bar condition is thermally neutral

Temperature rise at catalyst mid-bed

Axial Temperature Profiles for Preliminary Load Range Expansion Provide Confidence that Further Expansion is Possible

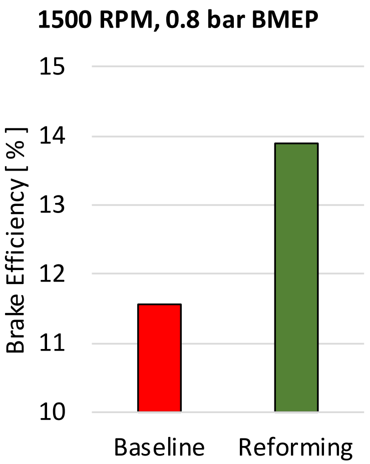
Accomplishments

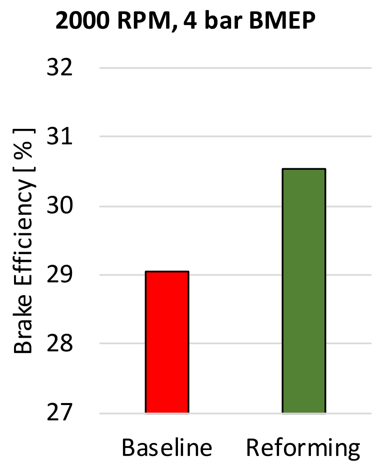


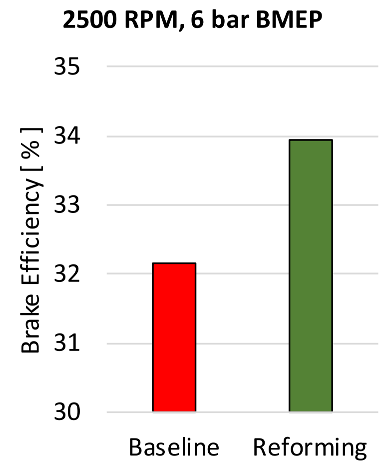
- Only 75°C difference in peak temperature
- Peak temperature controlled by oxygen present at catalyst inlet

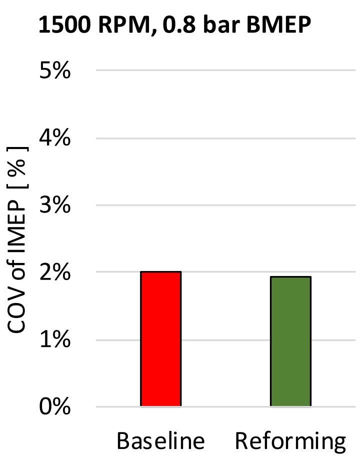
At Preliminary Load Range Expansion Points, Significant Increases in Brake Efficiency Realized While Maintaining Stability

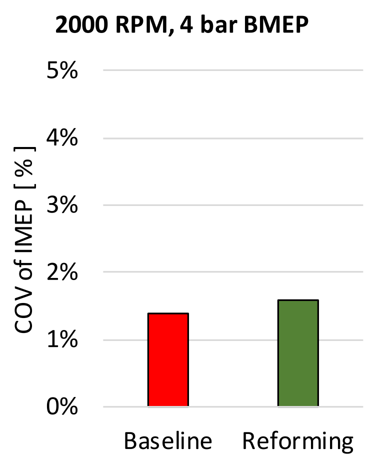
Accomplishments

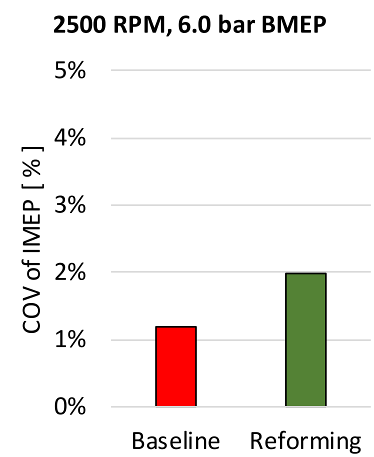






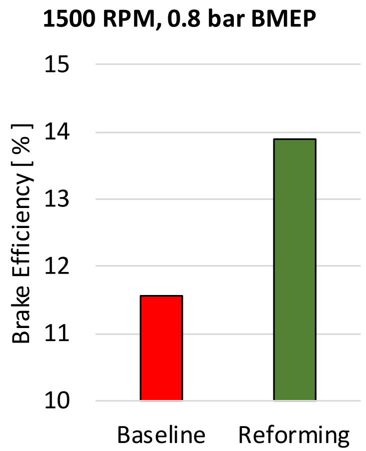


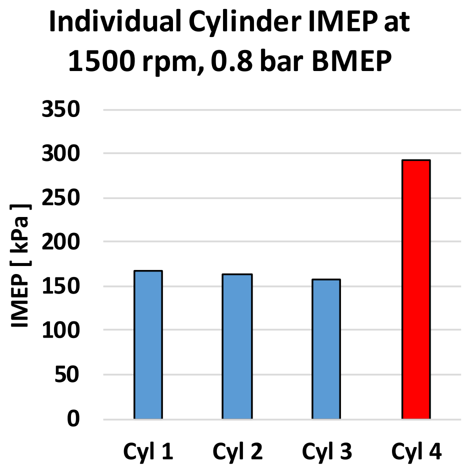


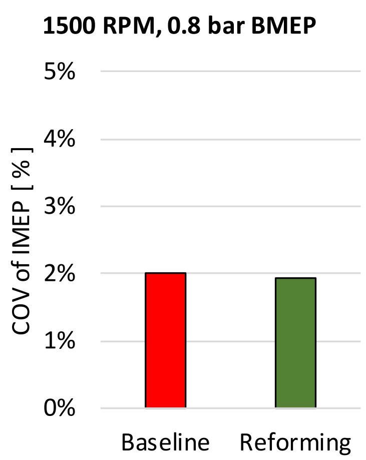


Light Load Condition Disallowed Load Balancing Between Cylinder due to Fuel in Trapped Residuals

Accomplishments







- Due to low exhaust temperature, reforming relied more strongly on POx reactions
  - High concentration of O_2 for high exotherm
  - Entirety of fuel for cyl 1-3 sent through reforming catalyst
- This results in a lot of fuel in cyl 4 trapped residuals
  - IMEP in cyl 4 could not be decreased sufficiently
  - Load could not be balanced across cylinders
- Oil dilution concerns with post-injection at higher loads
- **Desire to move away from post-injection in cylinder 4**

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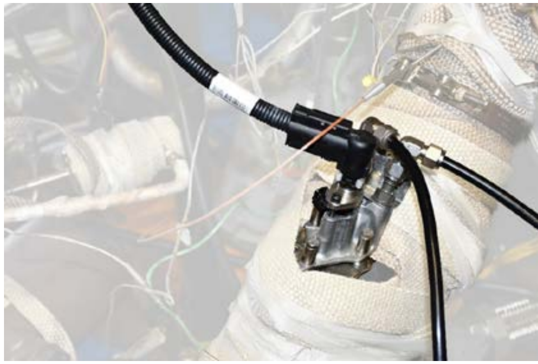
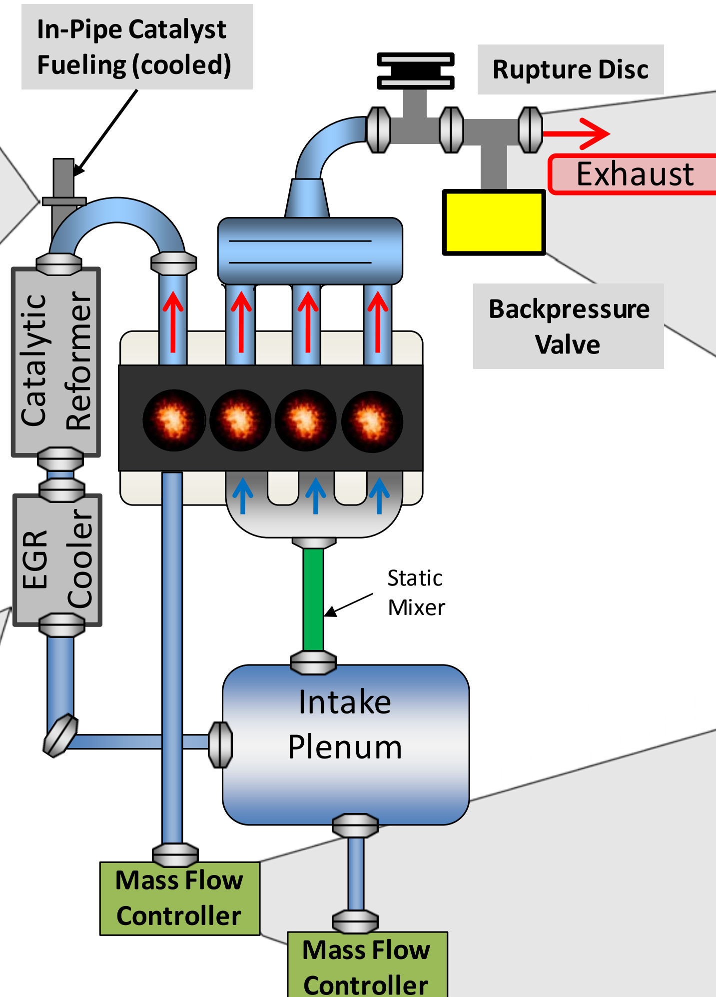
Experimental Modifications Implemented to Enable Boosted Operation and In-Pipe Reforming Catalyst Fueling

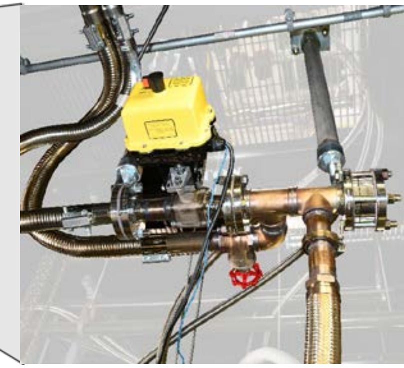
Accomplishments

Water-cooled housing for urea doser, fits Bosch PFI injector

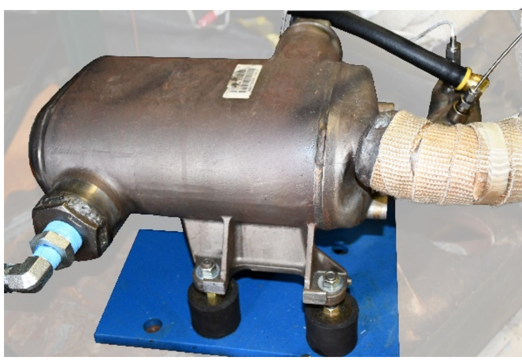




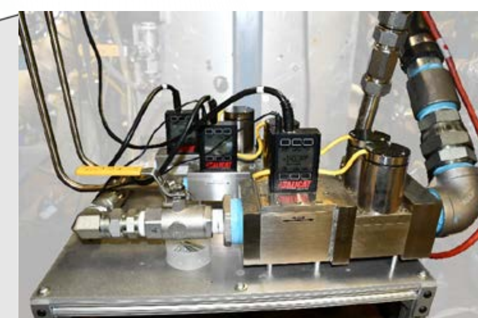
Backpressure Valve and Rupture Disc for Realistic Turbo Boundary Conditions



Boosted Operation Required Higher Capacity EGR Cooler (DDC Series 60)

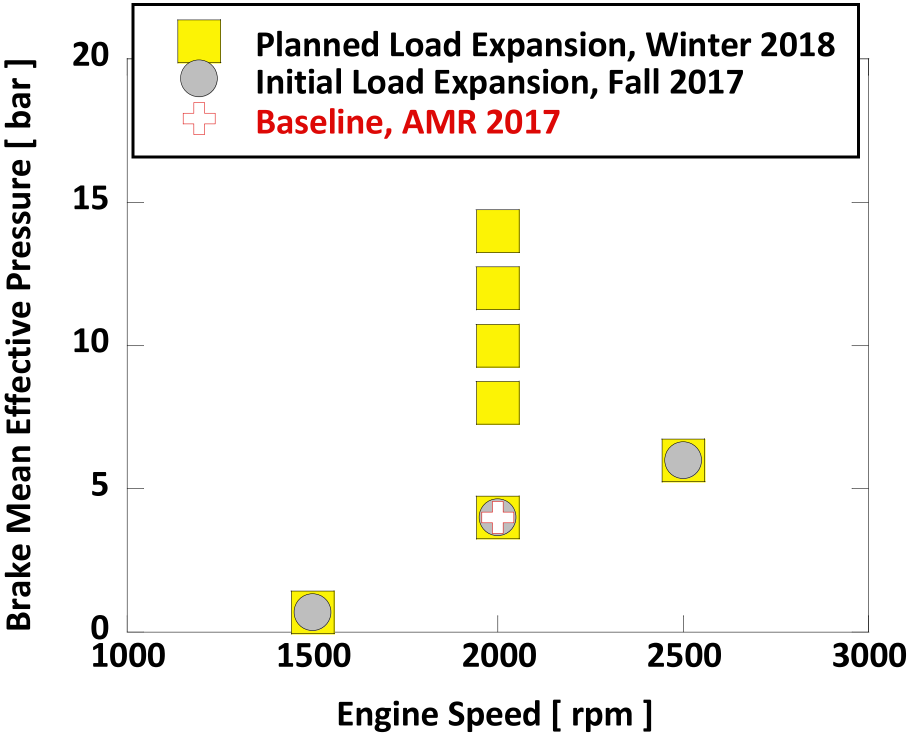


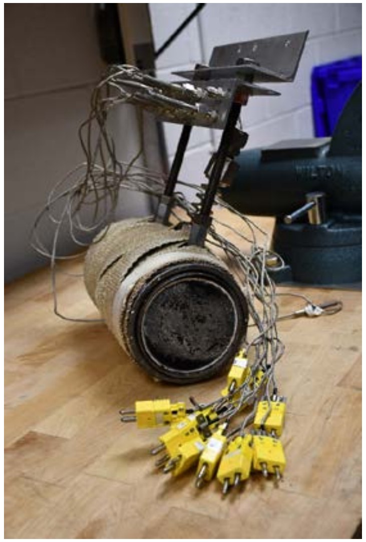
Bank of Mass Flow Controllers to Simulate Boost



Significant Progress Made on Load Range Expansion, but Experimental Events Resulted in Equipment Failure. Goal Not Yet Met.

Accomplishments



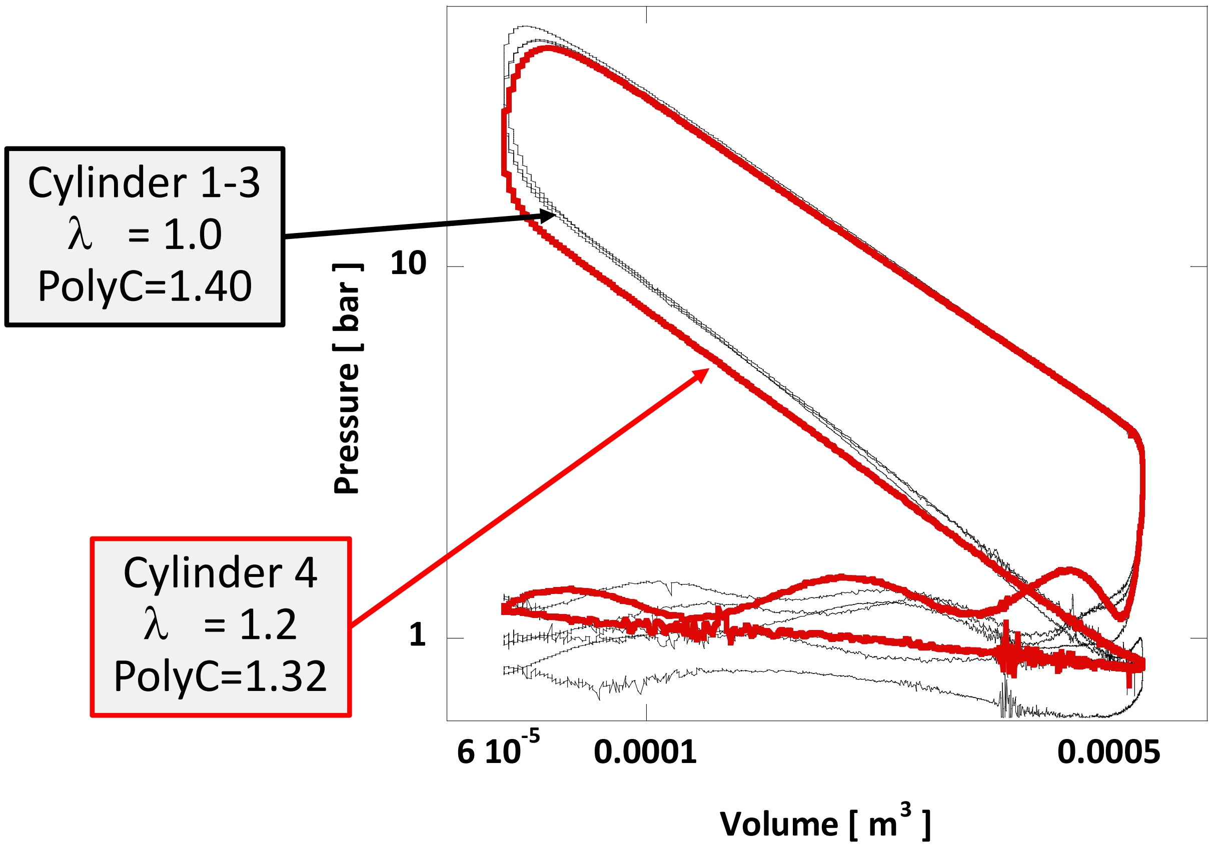


Despite severe overtemperature, zirconia mullite maintained structural integrity (i.e., no melted catalyst pieces recirculated to engine intake)

- Planned load expansion points with modified engine hardware aimed for boosted operation
  - Initial experiments at 2000 rpm 4 bar BMEP and 2500 rpm 6 bar BMEP were conducted successfully
  - Prior to going to boosted operation, cooling water connection in cell failed (~20 gal facility water in ~ 2 minutes)
  - Rushed shutdown led to overtemperature in catalyst, reached ~1400°C before thermocouple failure
  - Overtemperature occurred in EGR cooler immediately downstream of catalyst, melting a braze
  - EGR air system filled with water, including reforming catalyst

2017 AMR Reviewer Question: Could Efficiency be Higher with Lean Combustion?

Accomplishments



- Experimental measurements show that the polytropic coefficient is **higher** for the stoichiometric cylinders than the lean cylinder
- **What the heck is going on here???**

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Gamma Increases with Dilution Because Concentration of Fuel Decreases; Reforming Benefit 2x Lean (λ = 1.4) for Reactants!

Accomplishments

Stoichiometric Combustion: C_8H_{18} = 1.7 mol%

$C_8H_{18} + 12.5\ (O_2 + 3.76\ N_2) \rightarrow 8\ CO_2 + 9\ H_2O + 47\ N_2$

Lean Combustion (λ = 1.4): C_8H_{18} = 1.2 mol%

$C_8H_{18} + 17.5\ (O_2 + 3.76\ N_2) \rightarrow 8\ CO_2 + 9\ H_2O + 5\ O_2 + 65.8\ N_2$

EGR (40% EGR): C_8H_{18} = 1.2 mol%

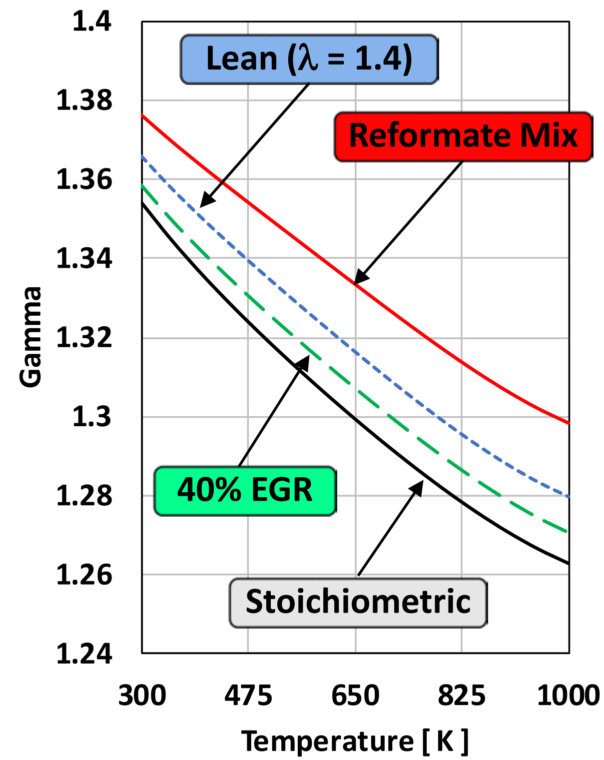
$\boxed{C_8H_{18}} + \boxed{12.5\ (O_2 + 3.76\ N_2)} + \boxed{2.98\ CO_2 + 3.35\ H_2O + 17.48\ N_2} \rightarrow$
$\boxed{10.98\ CO_2 + 12.35\ H_2O + 64.48\ N_2}$

Steam Reforming

$C_8H_{18} + 2.98\ CO_2 + 3.35\ H_2O + 17.48\ N_2 \rightarrow$
$\boxed{0.582\ C_8H_{18} + 2.98\ CO_2 + 17.48\ N_2 + 7.11\ H_2 + 3.35\ CO}$

Combustion with Reformate: C_8H_{18} = 0.6 mol%

$0.582\ C_8H_{18} + 2.98\ CO_2 + 17.48\ N_2 + 7.11\ H_2 + 3.35\ CO + 12.5\ (O_2 + 3.76\ N_2) \rightarrow$
$10.98\ CO_2 + 12.35\ H_2O + 64.48\ N_2$



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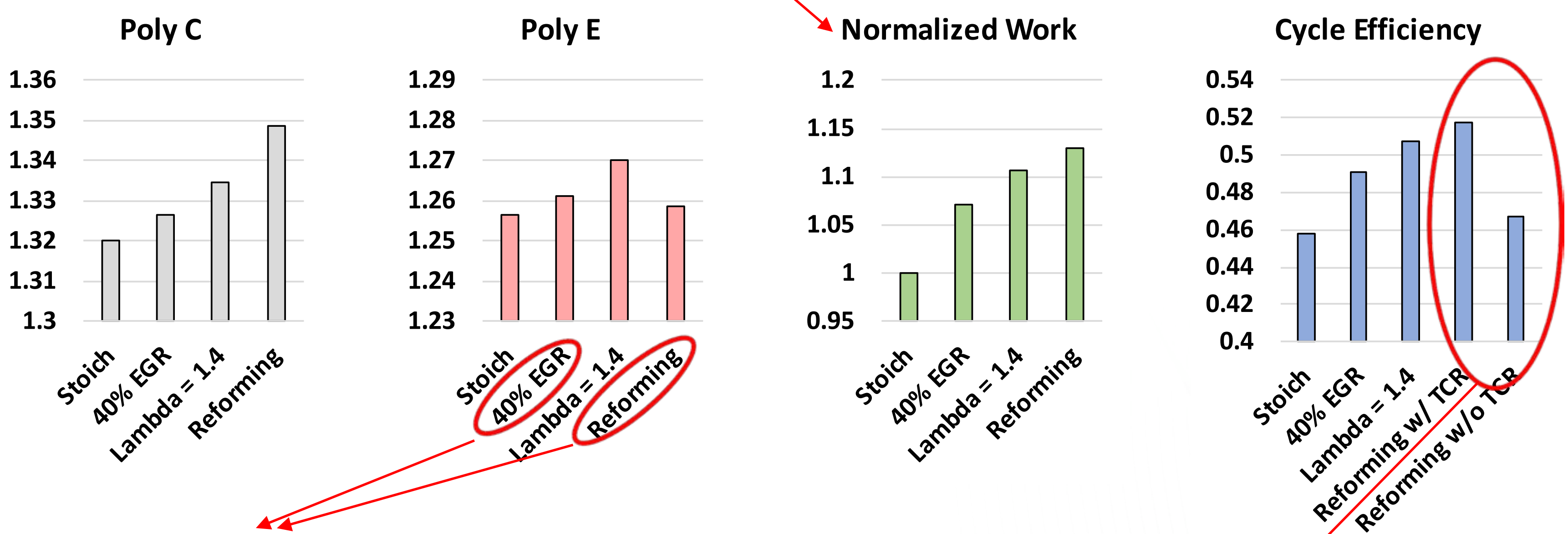
Thermodynamic Closed-Cycle Analysis Shows that Stoichiometric Efficiency with Reformate is Competitive with Lean Combustion

Accomplishments

- Chemkin used to evaluate closed cycle thermodynamics under adiabatic conditions
  - Weibe function used to impose common deflagration event for all conditions
  - All cases starting with the same iso-octane fuel energy

Includes TCR



- **Despite same composition, reforming case has lower Poly E**
- **Attributable to higher flame temperature for reformate**
  - **Lower molar expansion ratio**
  - **Lower exergy/enthalpy ratio**

- **Which LHV should we use???**
  - **Higher efficiency is iso-octane LHV**
  - **Lower efficiency is mixture LHV after reforming**

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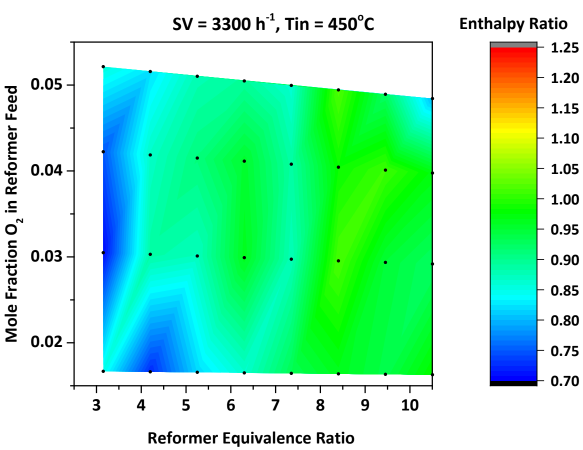
Related Project Aiming to Apply Same Reforming Strategy to Propane

Accomplishments

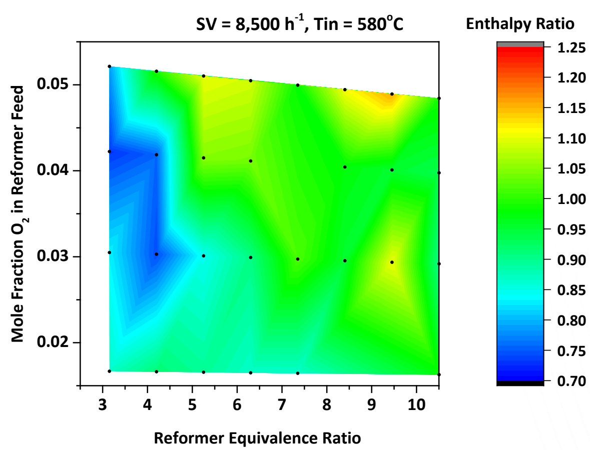
- Propane has higher H/C ratio than gasoline, making reforming thermodynamics more favorable
- Starting project with a flow-reactor investigation to characterize propane performance
  - Investigating a variety of inlet temperature/ space velocity
- Reforming thermodynamics become more favorable at higher load (higher temperature) conditions

	Regular Grade Gasoline	Propane
Fuel H/C Ratio	1.97	3.0
Steam Reforming H_2/CO Ratio	1.99	2.33
POx Reforming H_2/CO Ratio	0.99	1.33

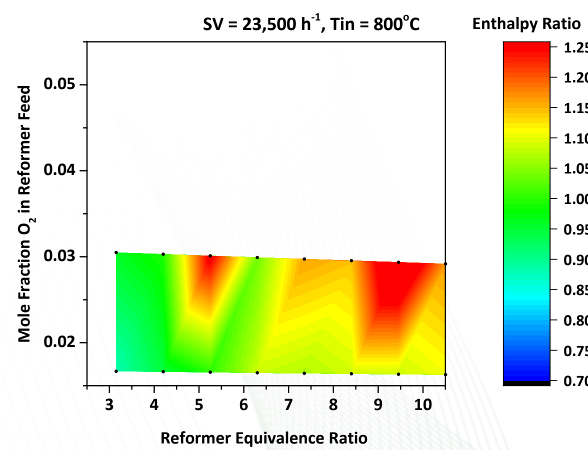
Replicates 1500 RPM, 0.7 bar



Replicates 2000 RPM, 4.0 bar



Replicates 2000 RPM, 14.0 bar



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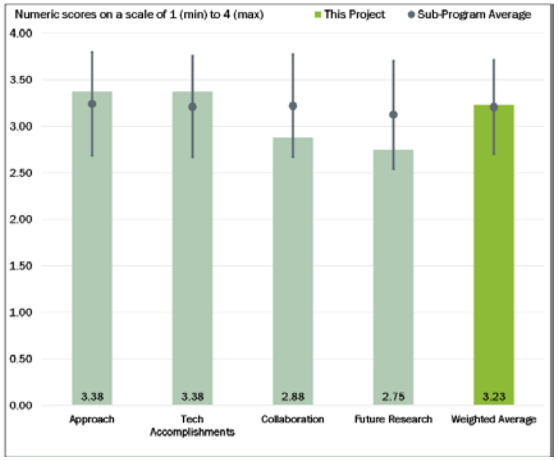
Four Reviewers Evaluated this Project in 2017
Overall Positive Comments with Room for Improvement

Several reviewers commented on the need for expanded speed/load range

We have made significant progress in this direction (1500 rpm, 0.8 bar BMEP; 2500 rpm, 6.0 bar BMEP). We are working towards higher load under boosted operating conditions and expect to have initial results by the end of FY18.



Two comments on emission barriers/opportunities, including cold-start

The focus on stoichiometric operation is to maintain compatibility with conventional 3-way catalysis. The low engine-out NOx emissions may have benefits under transient conditions. However, significant progress needs to be made before any transient testing. This is a stoichiometric SI engine, so cold-start could be done in a conventional manner (i.e., without reforming).

Collaborators listed, but no particular collaborator input is attributed to specific collaborators

Input from OEM partners has been to investigate light load (tip-out) and high load operation, with attention to combustion stability and emissions.

One reviewer requested additional information about the catalyst, and requested that we report the effects of different catalyst compositions

This catalyst was originally developed by Delphi for reforming purposes, and this project is building on prior industry expertise. Further catalyst development or testing different catalyst formulations is outside of the current project scope.

Collaborations

- Project direction from 2010 USCAR Colloquium
  http://feerc.ornl.gov/pdfs/Stretch_Report_ORNL-TM2010-265_final.pdf
- OEM Collaborations: one-on-one discussions, discussions of implementation barriers, feedback on results and future plans
  - Ford
  - Caterpillar
  - FCA
- Umicore – Providing pre-production Rh-based catalysts
- ANSYS (formerly Reaction Design) – CFD model development and technical assistance
- University of Michigan: Yan Chang is a UM student working on the project at ORNL for 2016, advised by Stani Bohac and André Boehman
- AEC Working Group bi-annual meetings
  - Mechanism for industry feedback
- University of Michigan: Galen Fisher advising on catalyst formulation and operating conditions through subcontract
- Related funds-in project with Aramco Services Co.
- Sandia National Laboratories: Historical collaboration with Isaac Ekoto (and Dick Steeper). Projects diverged this year, but technical discussions continue.

Remaining Barriers and Future Work

Remaining Barrier 1

This technology has only been demonstrated for a limited number of speed/load conditions. Engines are required to operate over a wider range of conditions.

Corresponding Future Work

Continue to experimentally expand the speed-load operating regime to both lighter loads and higher loads. Use flow reactor experiments to guide efficient reforming boundary conditions

Remaining Barrier 2

Unclear how much fuel-borne sulfur will limit the applicability of this technology.

Corresponding Future Work

Characterize the extent of sulfur deactivation at multiple speed-load operating conditions. If necessary, develop techniques to regenerate the catalyst with minimum fuel penalty.

Remaining Barrier 3

Combination of system thermodynamics, combustion processes, and energy losses is not fully understood.

Corresponding Future Work

Utilize 0-D thermodynamic modeling, 0-D kinetic modeling, 1-D gas exchange modeling, and 3D CFD modeling to provide a better understanding of the thermodynamics, reforming processes, and combustion processes.

Any proposed future work is subject to change based on funding level

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Summary

Relevance

Addressing research priorities called-out in the ACEC Roadmap for topic area 1:
a) low cost waste heat recovery, b) increased EGR tolerance, c) reduced complexity

Approach: Experimental and Modeling Efforts Grounded in Thermodynamics

- Synthetic exhaust flow reactor experiments define boundary conditions for high η reforming, TCR
- Operate engine to achieve efficient reforming boundary conditions in catalyst, pursue highest η
- 0-D thermodynamic through CFD modeling used to understand results, guide next steps

Accomplishments

- Published three articles in *Energy & Fuels* documenting reforming strategy from flow reactor to full scale multi-cylinder engine experiments
- Expanded speed-load range lower (1500 rpm, 0.8 bar BMEP) and higher (2500 rpm, 6.0 bar BMEP)
- Performed thermodynamic analysis of reformate on closed-cycle efficiency

Collaborations

- Ford, FCA, Caterpillar, Aramco Services Co., Umicore, Ansys, University of Michigan

Future Work

- Speed load expansion, sulfur tolerance, phenomenological modeling

Any proposed future work is subject to change based on funding level

Technical Backup Slides

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Hypothesis: Exergy/enthalpy ratio is related to the molar expansion ratio

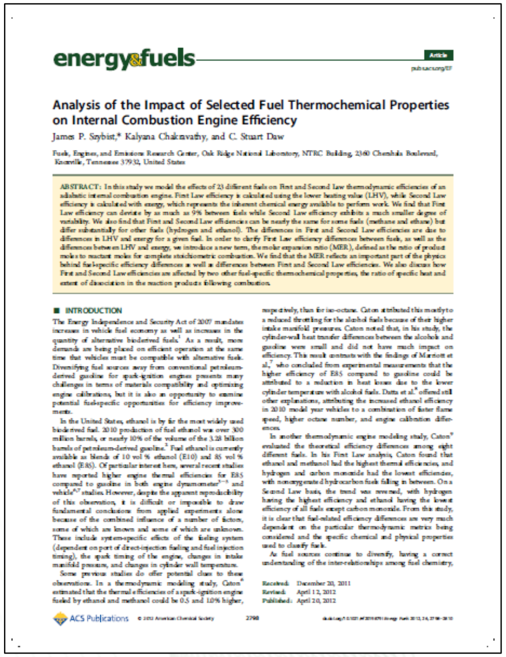
Backup (1/5)

Molar Expansion Ratio ≡ (moles products)/(moles reactants)

- Molar expansion ratio is dependent on fuel type

$CH_4 + 2\ (O_2 + 3.76\ N_2) \longrightarrow CO_2 + 2\ H_2O + 7.52\ N_2$	$n_{product}/n_{reactant} = 1.00$
$CH_3OH + 1.5\ (O_2 + 3.76\ N_2) \longrightarrow CO_2 + 2\ H_2O + 5.64\ N_2$	$n_{product}/n_{reactant} = 1.21$
$CO + 0.5\ (O_2 + 3.76\ N_2) \longrightarrow CO_2 + 1.88\ N_2$	$n_{product}/n_{reactant} = 0.85$

  - The molar change during combustion is not accounted for in the LHV measurement or the enthalpy of reaction
  - Change in the number of moles is accounted for in the entropy term, so it is included in exergy of reaction
- Current study is limited to stoichiometric combustion with air to maximize fuel differences in molar expansion ratio
  - Molar expansion ratio approaches unity with increasing dilution (lower equivalence ratio or higher EGR)


energy&fuels
Analysis of the Impact of Selected Fuel Thermochemical Properties on Internal Combustion Engine Efficiency
James P. Szybist,* Kalyana Chakravathy, and C. Stuart Daw

Szybist, J.P., K. Chakravathy, C.S. Daw. *Analysis of the Impact of Selected Fuel Thermochemical Properties on Internal Combustion Engine Efficiency.* Energy & Fuels, 2012, vol 26(5), pp. 2798-2810.

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Molar expansion ratio determines the extent of residual pressure available to perform work

Backup (2/5)

$CH_4 + 2(O_2 + 3.76\ N_2)$ | $CH_3OH + 1.5(O_2 + 3.76\ N_2)$ | $CO + 0.5(O_2 + 3.76\ N_2)$

Constant volume reactant chambers, Initial T = 100 C, Initial P = 1 atm

Q

P_{final} = 1 atm
No residual work potential

Q

P_{final} > 1 atm
Positive residual work potential

Q

P_{final} < 1 atm
Atmosphieric work potential

Final T = Initial T = 100 C

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Ideal Cycle Efficiency Analysis Shows Contribution of γ to Different Portions of the Cycle

Backup (3/5)

- Ideally you would want γ to be different for different parts of the cycle
  - Low γ for compression and expansion
  - High γ for heat addition
- This type of analysis is removed from reality and can produce efficiency > 100%
- In reality, γ is coupled throughout the cycle
  - Relationship of γ for different parts of the cycle changes with stoichiometric, lean, and reforming cases
  - More work is necessary to fully understand the tradeoffs


An assessment of thermodynamic merits for current and potential future engine operating strategies*

Martin L Wissink, Derek A Splitter, Adam B Dempsey, Scott J Curran, Brian C Kaul and Jim P Szybist

Abstract

Keywords

Introduction

$$\frac{dp}{d\theta} = \left(\frac{dp}{d\theta}\right)_Q + \left(\frac{dp}{d\theta}\right)_V + \left(\frac{dp}{d\theta}\right)_m + \left(\frac{dp}{d\theta}\right)_M \tag{2}$$

$$\left(\frac{dp}{d\theta}\right)_Q = \left(\frac{\gamma-1}{V}\right)\dot{Q} \tag{3}$$

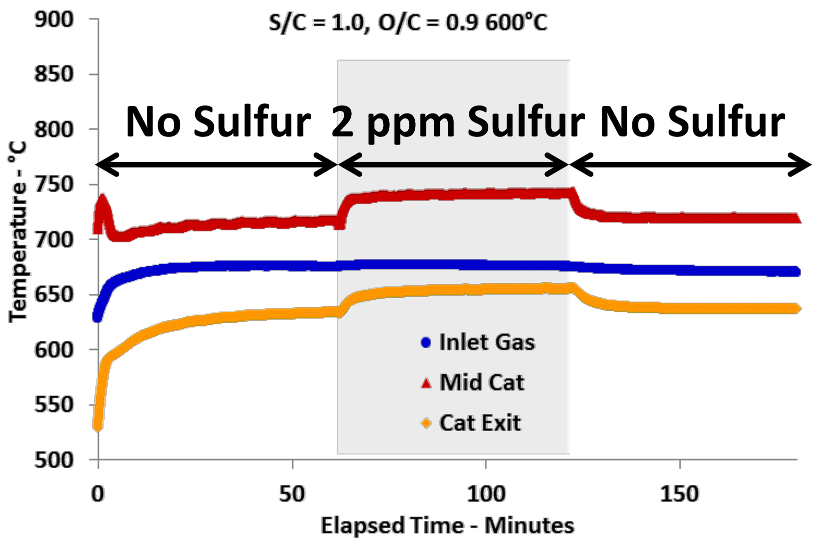
$$\left(\frac{dp}{d\theta}\right)_V = -\frac{\gamma p}{V}\frac{dV}{d\theta} \tag{4}$$

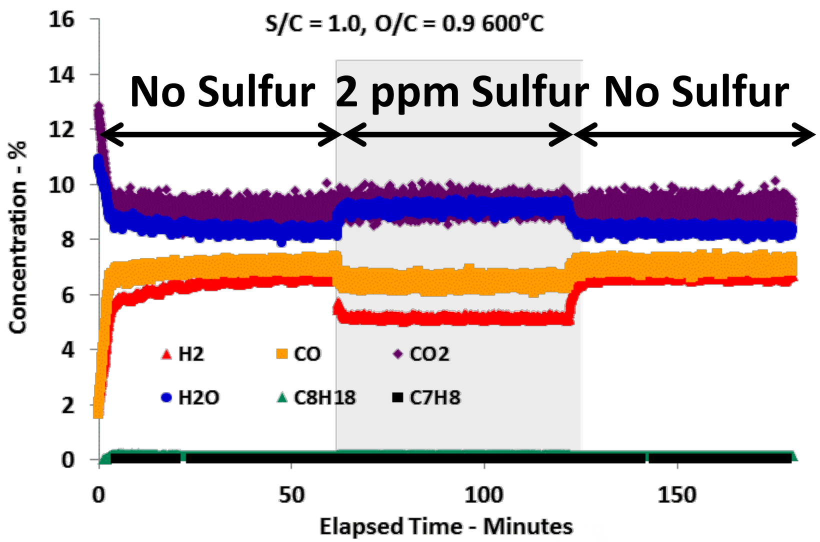
$$\left(\frac{dp}{d\theta}\right)_m = \left[\frac{\gamma p}{m} - \left(\frac{\gamma-1}{V}\right)(h-h_f)\right]\frac{dm}{d\theta} \tag{5}$$

$$\left(\frac{dp}{d\theta}\right)_M = -\frac{p}{M}\frac{dM}{d\theta} \tag{6}$$

Synthetic Exhaust Flow Reactor Demonstrates Sulfur Effect is Significant but Reversible

Backup (4/5)





- 2 ppm SO_2 introduced immediately upstream of reforming catalyst (represents fuel with 30 ppm S by mass)
- Steady conditions for 60 minutes show stable concentrations and temperatures
- Introduction of 2 ppm SO_2 causes increase in mid- and post-catalyst positions, accompanied by a reduction in reformate
- Near immediate recovery of reforming process when sulfur is removed

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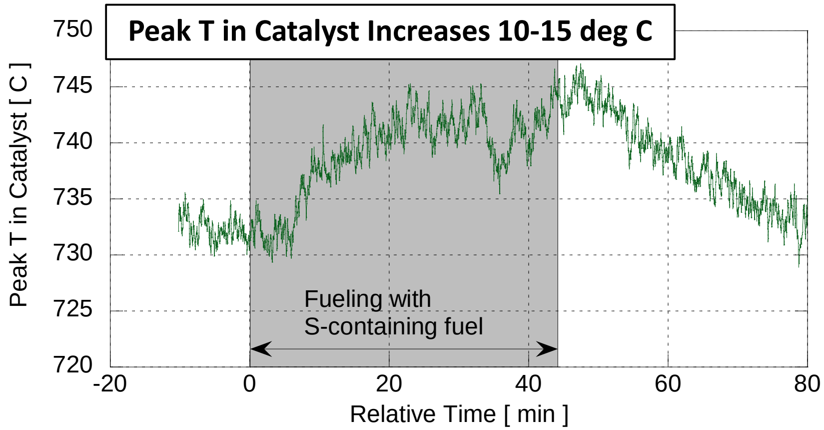
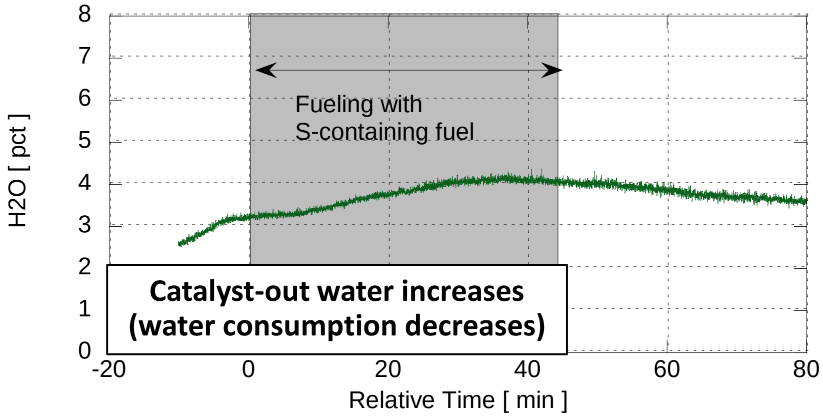
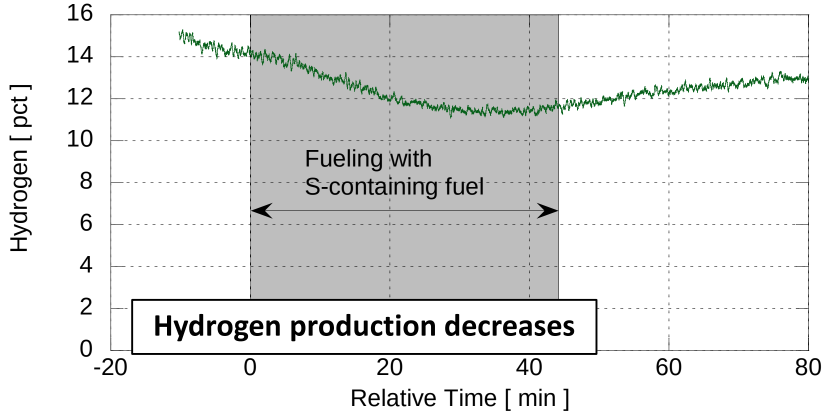
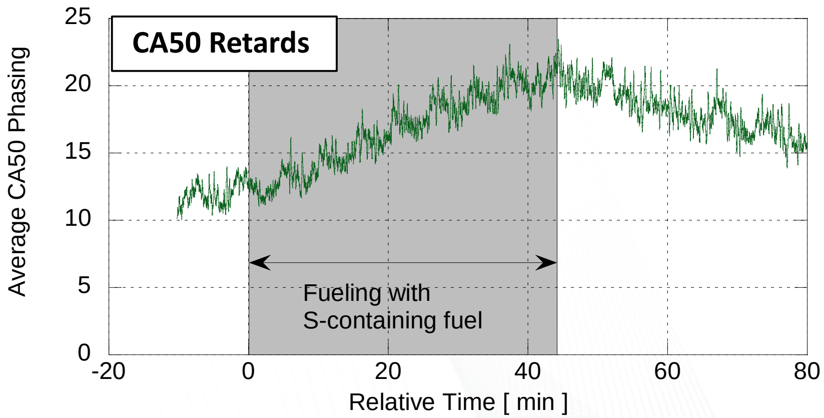
Preliminary Experiments at 1500 rpm, 0.8 bar BMEP Show Similar Trends as Flow Reactor but on Longer Timescales using 30 ppm S Fuel

Backup (5/5)









Sulfur poising to be revisited in more complete study later in FY18